(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization International Bureau



(43) International Publication Date 3 March 2005 (03.03.2005)

PCT

(10) International Publication Number WO 2005/019239 A2

(51) International Patent Classification7:

C07K

(21) International Application Number:

PCT/US2004/023092

(22) International Filing Date: 16 July 2004 (16.07.2004)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data: 60/488,415

18 July 2003 (18.07.2003) US

(71) Applicant (for all designated States except US): SMITHKLINE BEECHAM CORPORATION [US/US]; One Franklin Plaza, Philadelphia, PA 19101 (US).

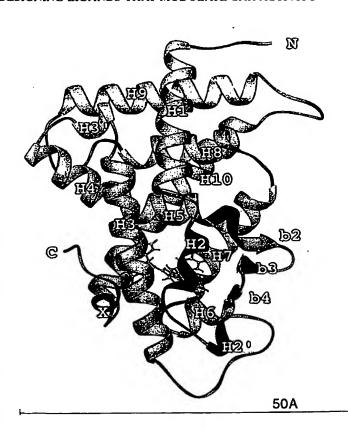
- (72) Inventors; and
- (75) Inventors/Applicants (for US only): COLLINS, Jon,

Loren [US/US]; GlaxoSmithKline, Five Moore Drive, PO Box 13398, Research Triangle Park, North Carolina 27709 (US). LAMBERT, III, Millard, Hurst [US/US]; GlaxoSmithKline, Five Moore Drive, PO Box 13398, Research Triangle Park, North Carolina 27709 (US). WISELY, George, Bruce [US/US]; GlaxoSmithKline, Five Moore Drive, PO Box 13398, Research Triangle Park, NC 27709 (US). XU, Robert [US/US]; GlaxoSmithKline, Five Moore Drive, PO Box 13398, Research Triangle Park, NC 27709 (US).

- (74) Agents: LEVY, David, J. et al.; GlaxoSmithKline, Five Moore Drive, PO Box 13398, Research Triangle Park, NC 27709 (US).
- (81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,

[Continued on next page]

(54) Title: CAR LIGAND-BINDING DOMAIN POLYPEPTIDE CO-CRYSTALLIZED WITH A LIGAND, AND METHODS OF DESIGNING LIGANDS THAT MODULATE CAR ACTIVITY



(57) Abstract: The present invention provides a crystalline form of a substantially pure constitutive androstane receptor (CAR) polypeptide. Also provided is a crystalline form of a substantially pure constitutive androstane receptor (CAR) polypeptide in complex with a ligand. Also provided are methods for generating the crystalline forms of the present invention and methods for identifying and designing CAR ligands and modulators. Also provided are scalable three-dimensional configurations of points and computer readable storage media containing digitally encoded structural data

MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SB, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GII, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CII, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

 without international search report and to be republished upon receipt of that report

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.